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Computing observables in curved multifield models of inflation

A guide (with code) to the transport method

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Abstract. We describe how to apply the transport method to compute inflationary observables in a broad range of multiple-field models. The method is efficient and encompasses scenarios with curved field-space metrics, violations of slow-roll conditions and turns of the trajectory in field space. It can be used for an arbitrary mass spectrum, including massive modes and models with quasi-single-field dynamics.

In this note we focus on practical issues. It is accompanied by a *Mathematica* code which can be used to explore suitable models, or as a basis for further development.

Keywords: inflation, multifield, initial conditions

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1 Introduction

Inflation [1–3] is a scenario for the very early universe according to which all large-scale structure originated as quantum fluctuations. This idea has been tested by increasingly detailed observations of anisotropies in the cosmic microwave background (CMB), and its broad predictions are now known to be compatible with their measured statistical properties [4]. This is a significant achievement which symbolises the maturation of modern cosmology into a precision science. However, despite this phenomenological success, it remains unclear whether or not the microphysical origin of inflation can be understood.

The simplest inflationary models comprise only a single scalar degree of freedom, taken to have a canonical kinetic term and a potential representing self-interactions. Minimal models of this kind are sufficient to obtain predictions consistent with observational constraints, and therefore are natural from the perspective of simplicity and economy. From the perspective of fundamental physics, however, their status is uncertain. If the inflationary scale is widely separated from the next relevant mass scale it may be natural to have only a single degree of freedom which is light by comparison, and a simple potential. But if the inflationary scale is not far below the next relevant scale—in particular, if the ultraviolet completion of the theory gives rise to multiple degrees of freedom which are light compared to the inflationary scale—then it may be that a model with *several* active scalar fields, coupled through a nontrivial potential or field-space metric, represents the most natural possibility.

Which of these choices is a better match for the large-scale structure we observe in our universe is a question to be resolved by measurement. To do so will require a clear understanding of the qualitative predictions which can be obtained in each scenario. In single-field potential-dominated models, an extended campaign of exploration has provided guidance about what can be expected. In this case the textbook approach to perturbations is applicable. Only a few e-folds around horizon exit are relevant; the decoupling principle tells us that effects long before horizon exit are negligible, and long after it the perturbations

become conserved. During these few e-folds we can assume the Hubble rate to be nearly constant and take the inflaton mass to be negligible.

In more complex models these simplifications no longer apply. If the field-space trajectory exhibits turns or other features around horizon exit then the calculation must usually begin far inside the horizon, tracking effects from perturbations with masses around the Hubble scale. Also, where multiple fields remain relevant after horizon exit we must continue to integrate until their observable effects are extinguished, possibly much later in the inflationary era or even long after it has ended. All but the heaviest modes will be relevant after horizon exit, including perturbations in the momenta.

These complexities frustrate the traditional textbook approach. If only a few of them are present it may still be possible to make analytic progress. But more generally, in models where they all occur, a numerical method is almost essential.

In this paper we show how the complexities introduced by many relevant scales can be accommodated, whether these scales are associated with masses in the particle spectrum or curvature scales in the field-space manifold. We illustrate our method with an explicit *Mathematica* implementation.¹ The version discussed here is available from transportmethod.com. We have attempted to simplify it as much as possible, with the intention of making it easy to follow. It can be used to compute the two-point function of inflationary fluctuations in a model with any number of fields and arbitrary potential and field-space metric. The numerical method (to be described in §2) is efficient, and therefore despite being implemented in *Mathematica* it is fast enough for practical model exploration. In situations where *Mathematica* is too slow or inconvenient, such as Monte Carlo sampling, it could serve as a reference implementation.²

Synopsis.—This paper is divided into four principal parts. In §2 we explain how to derive differential equations which express the time evolution of field-space correlation functions in the spatially flat gauge. We allow an arbitrary potential and field-space metric. With appropriate initial conditions this system of equations can be used to capture contributions (including quantum effects) from all mass scales as the fluctuations approach, pass through, and eventually evolve outside the Hubble length. We discuss the selection of initial conditions in §3.

In §4.1 we explain how to relate the flat-gauge field-space correlation functions to the statistical properties of the density perturbation, which is the observable quantity.

For a given model the major numerical uncertainty is the duration of nontrivial evolution on super-Hubble scales. In principle—no matter which scheme we use to compute the properties of observables—the equations for all inflationary perturbations should be integrated up to the last scattering surface, where they supply initial conditions for the cosmic

¹This implementation was originally developed to study a model of D-brane inflation [5]. The precise model is described in Ref. [6]. The Lagrangian is $\mathcal{L} = a^3 [\frac{1}{2} T_3 G_{ij} \dot{\phi}^i \dot{\phi}^j - V(\phi)]$ where a is the scale factor and T_3 is the brane tension. It consists of six fields ϕ^i representing coordinates in the throat of a Klebanov–Witten geometry which can be described by a noncompact conifold built over the five-dimensional $SU(2) \times SU(2)/U(1)$ coset space $T^{1,1}$. The details of this geometry are encoded in the nontrivial field-space metric G^{ij} . The potential includes stochastic contributions from the bulk and it consists of ~ 600 terms.

²Other general purpose codes exist. *FieldInf* is a Fortran code capable of computing the inflationary power spectrum in an N -field model with a nontrivial field-space metric [7–9]. *ModeCode* and *MultiModeCode* are similar Fortran codes designed (respectively) for single- and multiple-field models. They are restricted to a trivial field-space metric but emphasize Monte Carlo sampling [10–13]. *Pyflation* is a Python code which solves the Mukhanov–Sasaki equation to first-order in multiple-field models, and to second-order in single-field models [14–16]. Like *ModeCode* it is restricted to a trivial field-space metric.

microwave background anisotropies. In practice this is very onerous, and anyway would require us to integrate through epochs of cosmological history, such as reheating, about which we know nothing. To evade both these issues we must usually rely on the dynamics becoming ‘adiabatic’ at some point during inflation, or not long after—meaning that the isocurvature modes which can source time dependence of the density perturbation become exhausted, and it ceases to evolve. In §4.2 we discuss the issues which arise when trying to detect whether this limit has been reached.

Notation.—We set $c = \hbar = 1$ and express the gravitational coupling by the reduced Planck mass $M_{\text{P}}^{-2} \equiv 8\pi G$. Greek indices from the beginning of the alphabet, (α, β, \dots) label the species of light scalar fields; Greek indices from the middle of the alphabet (μ, ν, \dots) label spacetime dimensions. Spacetime indices are not needed except in Eq. (2.1).

2 Transport equations for correlation functions

An inflationary model with curved field space is governed by the action

$$S = \frac{1}{2} \int d^3x dt \sqrt{-g} \left\{ M_{\text{P}}^2 R - G_{\alpha\beta} g^{\mu\nu} \partial_\mu \phi^\alpha \partial_\nu \phi^\beta - 2V \right\}, \quad (2.1)$$

where $G^{\alpha\beta}$ is the field-space metric, V is the potential and $g^{\mu\nu}$ is the space-time metric. At background level we take this to be Robertson–Walker,

$$ds^2 = -dt^2 + a(t)^2 d\mathbf{x}^2, \quad (2.2)$$

where $a(t)$ is the scale factor. Both $G_{\alpha\beta}$ and V may be arbitrary functions of the fields ϕ^α provided they are compatible with field configurations which realize an inflationary epoch. The equation of motion for the unperturbed background fields is

$$\mathcal{D}_t \dot{\phi}^\alpha + 3H \dot{\phi}^\alpha + G^{\alpha\beta} V_\beta = 0, \quad (2.3)$$

where $V_\beta \equiv \partial_\beta V$, an overdot denotes partial differentiation with respect to cosmic time t and \mathcal{D}_t denotes a covariant time derivative, $\mathcal{D}_t X^\alpha \equiv \dot{X}^\alpha + \Gamma_{\beta\gamma}^\alpha \dot{\phi}^\beta X^\gamma$. The connexion $\Gamma_{\beta\gamma}^\alpha$ is the Levi–Civita connexion compatible with $G_{\alpha\beta}$.

Our aim is to study quantum fluctuations in this model, which are characterized by correlation functions of the independent degrees of freedom. Their precise identity is influenced by our choice of spacetime coordinates. In this paper we define time t so that slices of constant t have zero Ricci curvature, up to possible tensor modes which we neglect. In these coordinates the independent degrees of freedom are fluctuations $\delta\phi^\alpha$ in the fields, and the correlation functions characterizing quantum fluctuations are the n -point functions $\langle \delta\phi^\alpha(\mathbf{k}_1, t_1) \delta\phi^\beta(\mathbf{k}_2, t_2) \rangle$, $\langle \delta\phi^\alpha(\mathbf{k}_1, t_1) \delta\phi^\beta(\mathbf{k}_2, t_2) \delta\phi^\gamma(\mathbf{k}_3, t_3) \rangle$, and so on, together with their derivatives. For applications to inflation we typically require only the equal-time case where all t_i are evaluated at some common point t . The expectation value $\langle \dots \rangle$ is taken in a state which coincides with the Minkowski vacuum on deeply subhorizon scales.

2.1 Capturing physical effects from all mass scales

In order to ensure that we capture relevant physics from all mass scales, we begin the calculation sufficiently far inside the horizon that vacuum initial conditions apply. As we will show below, in de Sitter space all degrees of freedom of fixed mass become effectively *massless* on

subhorizon scales, so—irrespective of the mass spectrum—we can obtain initial conditions for each n -point function to arbitrary accuracy by beginning the calculation sufficiently long before horizon exit. The details are discussed in §3.

We then apply the in–in formalism to derive an evolution equation for each n -point function, incorporating all masses and (in principle) quantum effects.³ These evolution equations are equivalent to the separation into in–out expectation values and subsequent Feynman expansion used by Maldacena and later authors to obtain analytic estimates of the correlation functions [19]. But unlike the expansion into diagrams they do not involve Green’s functions—only ordinary differential equations. Therefore they constitute a differential formulation of the theory rather than an integral one, and can be handled by conventional ODE solvers.

Perturbed action.—To second order in amplitude, the action governing small fluctuations $\delta\phi^\alpha$ around a homogeneous solution $\phi^\alpha(t)$ of (2.1) can be written [20, 21]

$$S \supseteq \frac{1}{2} \int \frac{d^3k}{(2\pi)^3} dt a^3 \left\{ G_{\alpha\beta} [\mathcal{D}_t \delta\phi^\alpha(\mathbf{k})] [\mathcal{D}_t \delta\phi^\beta(-\mathbf{k})] - \left(\frac{k^2}{a^2} G_{\alpha\beta} + M_{\alpha\beta} \right) \delta\phi^\alpha(\mathbf{k}) \delta\phi^\beta(-\mathbf{k}) \right\}, \quad (2.4)$$

where the effective mass matrix $M_{\alpha\beta}$ is defined by

$$M_{\alpha\beta} \equiv V_{\alpha;\beta} - R_{\alpha\lambda\mu\beta} \dot{\phi}^\lambda \dot{\phi}^\mu - \frac{1}{a^3 M_{\text{P}}^2} \mathcal{D}_t \left(a^3 \frac{\dot{\phi}_\alpha \dot{\phi}_\beta}{H} \right). \quad (2.5)$$

In this expression $V_{\alpha;\beta} \equiv \partial_\beta V_\alpha - \Gamma_{\alpha\beta}^\gamma V_\gamma$ is the covariant derivative of V_α , and $R_{\alpha\lambda\mu\beta}$ is the Riemann tensor built from the metric connexion $\Gamma_{\beta\gamma}^\alpha$. As before, an overdot denotes a partial derivative with respect to t . Both $M_{\alpha\beta}$ and $G_{\alpha\beta}$ should be evaluated on the homogeneous background $\phi^\alpha(t)$.

Our formalism requires only Eq. (2.4). It is not necessary that it derives from an action of the form (2.1) which controls both the background and fluctuations. In particular, it may happen that (2.4) applies to the fluctuations in scenarios which have a more general noncanonical kinetic structure than (2.1). (Note, however, that (2.4) is not sufficiently general to cover fluctuations in a $P(X, \phi)$ model where the Lorentz symmetry between time- and space-derivative terms would be broken by a nontrivial sound speed c_s^2 .) Where Eq. (2.4) applies, our evolution equations for the two-point correlation functions apply likewise. They may be used to compute the properties of the fluctuations, although the background equations [Eqs. (2.8)–(2.9) below] would require modification.

The constituents of Eq. (2.4), including the perturbation $\delta\phi^\alpha$, transform covariantly under a change of coordinates in field space. This implies that $\delta\phi^\alpha$ must be understood as a tangent vector, not a coordinate displacement. The necessary formalism underlying this interpretation was given by Gong & Tanaka [22]; see also Ref. [20]. To lowest order in $\delta\phi^\alpha$ this makes no difference, but it would become important in any attempt to extend (2.4) to third order or above.

Quantization.—To quantize the fluctuations we define a momentum δp_α by the rule $\delta p_\alpha = \delta S / \delta (\mathcal{D}_t \delta\phi^\alpha)$. Then $\delta\phi^\alpha$ and δp_α are to be treated as operators satisfying the commutation

³In principle the evolution equations contain the same information as the loop expansion of conventional perturbation theory, but not nonperturbative information such as instanton effects. In practice one must truncate each evolution equation, which is equivalent to truncating the loop expansion at a particular order. In this paper we work to tree level, which is already sufficient to capture those quantum interference effects around horizon crossing which determine the ‘quantum’ part of the Feynman calculation [17, 18].

relation

$$[\delta\phi^\alpha(\mathbf{k}_1), \delta p_\beta(\mathbf{k}_2)] = i(2\pi)^3 \delta_\beta^\alpha \delta(\mathbf{k}_1 + \mathbf{k}_2) \quad (2.6)$$

and the Hamiltonian is

$$\mathcal{H} = \int \frac{d^3k}{(2\pi)^3} \left([\mathcal{D}_t \delta\phi^\alpha(\mathbf{k})] \delta p_\alpha(-\mathbf{k}) - \mathcal{L} \right), \quad (2.7)$$

where \mathcal{L} is the Lagrangian density appearing in (2.4). The equations of motion for $\delta\phi^\alpha$ and δp_α can be determined from \mathcal{H} via the Heisenberg equation.

In practice it is numerically more convenient to integrate in terms of the e-folding number $dN = H dt$ rather than dt itself. To do so at the level of the background we define

$$\pi^\alpha \equiv \frac{d\phi^\alpha}{dN} = \mathcal{D}_N \phi^\alpha, \quad (2.8)$$

in which it should be remembered that ϕ^α (being a coordinate) behaves like a field-space *scalar*, whereas π^α (being the derivative of a coordinate) behaves like a field-space *vector*. The background equations of motion now comprise (2.8) together with an evolution equation for π^α ,

$$\mathcal{D}_N \pi^\alpha = (\epsilon - 3)\pi^\alpha - \frac{G^{\alpha\beta} V_\beta}{H^2}. \quad (2.9)$$

To effect a similar change for the quantized perturbations we define

$$\delta\pi_\alpha \equiv \frac{\delta p_\alpha}{Ha^3} = \mathcal{D}_N \delta\phi_\alpha, \quad (2.10)$$

where the index on $\delta\phi^\alpha$ should be lowered using the metric $G_{\alpha\beta}$. Because the operations of taking covariant perturbations and covariant time-derivatives commute, it follows that $\delta(\mathcal{D}_N \phi^\alpha) = \mathcal{D}_N \delta\phi^\alpha$, and therefore $\delta\pi_\alpha$ can be regarded as an honest perturbation to the rescaled background field (2.8) [22]. This identification is not spoiled by raising or lowering the index because the metric is covariantly constant. The equations of motion for $\delta\phi^\alpha$ and $\delta\pi^\alpha$ can now be written

$$\mathcal{D}_N \delta\phi^\alpha = -\frac{i}{H} [\delta\phi^\alpha, \mathcal{H}] \quad (2.11a)$$

$$\mathcal{D}_N \delta\pi^\alpha = -\frac{i}{H} [\delta\pi^\alpha, \mathcal{H}] + (\epsilon - 3)\delta\pi^\alpha. \quad (2.11b)$$

Similar operator equations will hold in the quantum theory, possibly modified by renormalizations required to define composite operators appearing in the commutators $[\cdot, \mathcal{H}]$. Because these are operator equations they hold for any insertion of $\delta\phi^\alpha$ or $\delta\pi^\alpha$ in a correlation function, provided it is not coincident with any other operator. If we work only to tree-level the complexities associated with renormalization are not needed, and we can work directly with the bare equations. The noncanonical term in the evolution equation for $\delta\pi^\alpha$ arises from the explicit time-dependent factors a^3 and H which appear in (2.10).

Transport equations.—Salopek, Bond & Bardeen pointed out that a single solution of the $2N$ differential equations (2.11) is not sufficient to compute the two-point correlation functions [23]. A single solution characterizes only how the late-time $\delta\phi^\alpha$ and $\delta\pi^\alpha$ perturbations respond to a particular linear combination of fluctuations at an earlier time, and to compute a correlation function we must know how the late-time perturbations respond to

an arbitrary early-time perturbation. This entails calculating $2N$ solutions of (2.11), one for each independent initial condition.

Various formalisms exist to compute the required solutions.⁴ We choose to use the operator equations (2.11) to obtain evolution equations for each n -point function. There is no loss of information compared with solving for the field modes themselves, because only the correlation functions are meaningful: the predictions of an inflationary model are statistical, and are obtained by interpreting the correlation functions as ensemble averages and supposing that our particular universe is typical.

In this paper we deal only with the equal-time two-point functions, which are sufficient to obtain lowest-order inflationary observables. There are four such functions: $\langle \delta\phi^\alpha \delta\phi^\beta \rangle$, $\langle \delta\pi^\alpha \delta\phi^\beta \rangle$, $\langle \delta\phi^\alpha \delta\pi^\beta \rangle$, and $\langle \delta\pi^\alpha \delta\pi^\beta \rangle$. To compress notation we denote a generic perturbation such as $\delta\phi^\alpha$ or $\delta\pi^\alpha$ as X^a . The index a ranges over the field and momentum perturbations for each species α . To distinguish these we continue to label field perturbations by α, β, \dots , but add a bar to the species label for a momentum perturbation, giving $\bar{\alpha}, \bar{\beta}, \dots$, and so on. A generic equal-time two-point function can now be written

$$\langle X^a(\mathbf{k}_1) X^b(\mathbf{k}_2) \rangle = (2\pi)^3 \delta(\mathbf{k}_1 + \mathbf{k}_2) \frac{\Sigma^{ab}}{k^3}. \quad (2.12)$$

The evolution equation for Σ^{ab} follows from Ehrenfest's theorem,

$$\mathcal{D}_N \langle X^a X^b \rangle = \langle (\mathcal{D}_N X^a) X^b \rangle + \langle X^a (\mathcal{D}_N X^b) \rangle. \quad (2.13)$$

This argument, valid for quantum-mechanical correlation functions, was given by Mulryne [32]. It entails solving of order $2N \times 2N$ differential equations with a single initial condition, consistent with the counting argument given above. Using the symmetries of $\langle X^a X^b \rangle$ shows that there are $3N(N+1)/2$ independent equations, assuming that we use the Weyl-ordered correlation functions to be defined in §3.1.

Up to this point our treatment has been exact, except that by implicitly computing expectation values in a single state, corresponding to a fixed field configuration, we have restricted attention to what is visible in perturbation theory in the vicinity of that configuration. Therefore Eqs. (2.11) and (2.13) contain the same information as the loop expansion, and Eqs. (2.11) must contain information about all orders in interactions, represented by terms of all orders in $\delta\phi^\alpha$ and $\delta\pi^\alpha$ on the right-hand side. Hence

$$\mathcal{D}_N X^a = u^a_b X^b + \dots, \quad (2.14)$$

where u^a_b is a matrix which can be computed⁵ using Eqs. (2.11), and ‘ \dots ’ denotes terms of order $X^a X^b$ and higher which we have omitted. Neglecting these terms corresponds to

⁴Salopek, Bond & Bardeen decomposed the late-time fluctuations into a linear combination of creation–annihilation operators for the early-time fields, and solved for the resulting mixing matrix [23]. See Ringeval [9], Huston & Christopherson [16] and Price, Frazer, Xu, Peiris & Easter [13] for recent applications. McAllister, Renaux-Petel and Xu solved Eqs. (2.11) explicitly, once for each independent initial condition [24]. Lalak, Langlois, Pokorski & Turzyski applied a method very similar to that proposed by Salopek et al. [25]. The Γ -matrix or ‘propagator’ introduced in Ref. [26] is of a similar kind. Rigopoulos, Shellard & van Tent [27, 28] elaborated a formalism due to Groot Nibbelink & van Tent [29], using a basis aligned with the instantaneous background trajectory. This can reduce the number of integrations required if we are prepared to give up knowledge of the isocurvature modes. A similar approach was used by Peterson & Tegmark [30, 31].

⁵As explained above, we are neglecting renormalization and operator mixing effects which may be generated by the proper definition of composite operators beyond tree level.

working at tree-level in the loop expansion. On the left-hand side, the covariant derivative \mathcal{D}_N acts on the generic label a appropriately for the ‘barred’ and ‘unbarred’ types, so that $\mathcal{D}_N X^\alpha = \partial_N X^\alpha + \Gamma_{\beta\gamma}^\alpha \pi^\beta X^\gamma$ and $\mathcal{D}_N X^{\bar{\alpha}} = \partial_N X^{\bar{\alpha}} + \Gamma_{\beta\gamma}^\alpha \pi^\beta X^{\bar{\gamma}}$.

Combining Eqs. (2.12), (2.13) and (2.14) gives

$$\mathcal{D}_N \Sigma^{ab} = u^a{}_c \Sigma^{cb} + u^b{}_c \Sigma^{ac} + \dots, \quad (2.15)$$

which we describe as the *transport equation* for Σ^{ab} [33, 34]. The curved field-space version derived here was first given in Ref. [20]. Comparison with Eqs. (2.4), (2.7) and (2.11) shows that the components of $u^a{}_b$ satisfy

$$\begin{aligned} u^\alpha{}_\beta &= 0 \\ u^\alpha{}_{\bar{\beta}} &= \delta_\beta^\alpha \\ u^{\bar{\alpha}}{}_\beta &= -\delta_\beta^\alpha \frac{k^2}{a^2 H^2} - \frac{M^\alpha{}_\beta}{H^2} \\ u^{\bar{\alpha}}{}_{\bar{\beta}} &= (\epsilon - 3) \delta_{\bar{\beta}}^{\bar{\alpha}}. \end{aligned} \quad (2.16)$$

Mass dependence.—The epoch of ‘horizon exit’ occurs when the physical wavelength of order a/k associated with the comoving wavenumber \mathbf{k} becomes comparable to the Hubble length $1/H$. At this time the ratio k/aH is of order unity. Prior to horizon exit $k/aH \gtrsim 1$, and provided we are not too close to the start of the inflationary era it will be possible to find a point where $(k/aH)^2$ is much larger than any component of the effective mass matrix $M^\alpha{}_\beta/H^2$. If we choose to begin the calculation at or before this time then all fields can be treated as effectively massless. Where horizon exit is too close to the start of inflation it will not be possible to make $M^\alpha{}_\beta/H^2$ entirely negligible, and we must find some other way to supply initial conditions, presumably depending on the pre-inflationary history. The calculation then becomes model dependent, but not harder as a matter of principle. In this paper we will not consider such possibilities.

If H and $M^\alpha{}_\beta$ are nearly constant and the components of $M^\alpha{}_\beta$ are at most a few orders of magnitude larger than H^2 then the point where all fields become effectively massless might lie no more than $N \gtrsim 3$ e-folds before horizon exit. At the other extreme, if $H \approx 10^{12}$ GeV (corresponding to roughly GUT-scale inflation) but $M^\alpha{}_\beta$ contains terms of order M_P then it could be necessary to begin $N \gtrsim 14$ e-folds before horizon exit. These estimates require refinement if H or $M^\alpha{}_\beta$ vary significantly (see §3.2 for a numerical prescription). After horizon exit, k/aH becomes exponentially small and all but the most suppressed contributions to $M^\alpha{}_\beta$ will be relevant.⁶

Eqs. (2.15) and (2.16) provide a unified way to study both sub- and super-horizon regimes while retaining all relevant contributions to $M^\alpha{}_\beta$. In the literature these regimes are sometimes associated with ‘quantum’ and ‘classical’ behaviour, but both of these descriptions

⁶In certain models there may be a superheavy scale $\gg H$ above which all modes can be neglected: the fluctuations in these modes decay rapidly because of their large mass. Also, the potential for a superheavy field is so steep that the background trajectory can be assumed to make no excursion in its direction.

Although such a superheavy scale is normally assumed to exist, it has recently been appreciated that it is not straightforward to decide how large a mass is required before a field-space direction is negligible in this sense. The effect of massive modes is suppressed by inverse powers of the heavy mass M , but the rate of turn of the trajectory can be large. This gives a large number which can compensate for the smallness of $1/M$, making the direction more relevant than it would appear. A literature has developed to study these effects; for example, see Refs. [35, 36].

are marginally misleading. In the subhorizon era we work only to tree level and therefore true quantum effects are absent, but the initial conditions are quantum-mechanical and mix growing- and decaying-mode solutions for the elementary wavefunctions which contribute to Σ^{ab} . It is the interference between these modes which determines the higher-order correlations imprinted around the time of horizon exit. In the superhorizon era the evolution becomes classical in the restricted sense that decaying solutions die away.

‘In–in’ and ‘ δN ’ limits.—Once suitable initial conditions have been selected, it does not matter what spectrum of mass scales exists in M^α_β , or whether H varies significantly during or after the epoch of horizon exit. Eqs. (2.15)–(2.16) provide an alternative to the full diagrammatic description of the in–in formalism, but one which is equivalent. No further approximations are required. To determine the evolution of each correlation function we need only integrate the transport equation.

When written in this form it is simple to obtain the connexion between the in–in formalism and the ‘separate universe picture’, which gives an intuitive classical description of the evolving fluctuations on superhorizon scales [17, 21, 37–40]. In this limit the transport equation becomes a Jacobi equation describing the dispersion of neighbouring inflationary trajectories in field space and can be integrated analytically to produce the well-known ‘ δN ’ Taylor expansion [20, 26, 32].⁷

Scale dependence of two-point function.—A similar transport equation can be obtained for the scale dependence of the 2-point correlation function, which we measure using the matrix

$$n^{ab} \equiv \frac{d\Sigma^{ab}}{d \ln k}. \quad (2.17)$$

A transport equation for n^{ab} can be obtained by differentiating Eq. (2.15) [42]

$$\mathcal{D}_N n^{ab} = \frac{d}{d \ln k} \mathcal{D}_N \Sigma^{ab} = u^a{}_c n^{cb} + u^b{}_c n^{ac} + \frac{du^a{}_c}{d \ln k} \Sigma^{cb} + \frac{du^b{}_c}{d \ln k} \Sigma^{ac}. \quad (2.18)$$

Tensor modes⁸.—Tensor perturbations γ_{ij} are transverse, traceless perturbations of the spatial metric representing gravitational waves. Up to second order in amplitude their fluctuations are controlled by the action

$$S \supseteq \frac{M_{\text{P}}^2}{8} \int d^3x dt a^3 \left\{ \dot{\gamma}_{ij} \dot{\gamma}_{ij} - \frac{k^2}{a^2} \gamma_{ij} \gamma_{ij} \right\} \quad (2.19)$$

where the Latin indices i, j run over the three spatial coordinates. To obtain scalar equations it is convenient to decompose γ_{ij} into a basis of polarizations. In Fourier space this gives

$$\gamma_{ij}(\mathbf{x}) = \int \frac{d^3k}{(2\pi)^3} \sum_s \gamma_s(\mathbf{k}) e_{ij}^s(\mathbf{k}) e^{i\mathbf{k} \cdot \mathbf{x}} \quad (2.20)$$

where the polarization sum s runs over the orthogonal states $s \in \{+, \times\}$. The corresponding polarization matrices are traceless and satisfy $k_i e_{ij}^s(\mathbf{k}) = 0$, and are normalized so that $e_{ij}^s e_{ij}^{s'} = 2\delta^{ss'}$. Each polarization $M_{\text{P}} \gamma_s(\mathbf{k}) / \sqrt{2}$ behaves as a canonically-normalized free scalar

⁷It is possible, but substantially more complex, to see how the ‘ δN ’ description emerges from the diagrammatic expansion [41].

⁸The calculations reported in this section were performed in collaboration with Sean Butchers.

field. Therefore the two-point correlation function of tensor perturbations is insensitive to the mass hierarchies of the system.

To write an evolution equation for it we define the tensor momentum $\pi_s = d\gamma_s/dN$ and collect γ_s and π_s into a two-component vector $\gamma_s^{\mathfrak{a}} = (\gamma_s, \pi_s)$. The labels $\mathfrak{a}, \mathfrak{b}, \dots$, range over the tensor polarization and its momentum. We write the two-point function of $\gamma_s^{\mathfrak{a}}$ as

$$\langle \gamma_s^{\mathfrak{a}}(\mathbf{k}_1) \gamma_{s'}^{\mathfrak{b}}(\mathbf{k}_2) \rangle = (2\pi)^3 \delta_{ss'} \delta(\mathbf{k} + \mathbf{k}') \Gamma^{\mathfrak{ab}}. \quad (2.21)$$

It follows directly from Eqs. (2.15) and (2.16) that $\Gamma^{\mathfrak{ab}}$ obeys the transport equation

$$\frac{d\Gamma^{\mathfrak{ab}}}{dN} = w_{\mathfrak{c}}^{\mathfrak{a}} \Gamma^{\mathfrak{cb}} + w_{\mathfrak{c}}^{\mathfrak{b}} \Gamma^{\mathfrak{ac}} + \dots \quad (2.22)$$

where (with no summation implied) $w^\gamma_\gamma = 0$, $w^\gamma_\pi = 1$, $w^\pi_\gamma = -k^2/(a^2 H^2)$ and $w^\pi_\pi = \epsilon - 3$.

Following the same procedure that lead to Eq. (2.18), it is straightforward to compute the scale dependence of the tensor spectrum. Defining the quantity

$$n_{\text{T}}^{\mathfrak{ab}} \equiv \frac{d\Gamma^{\mathfrak{ab}}}{d \ln k}, \quad (2.23)$$

it follows that its equation of motion is

$$\frac{dn_{\text{T}}^{\mathfrak{ab}}}{dN} = w_{\mathfrak{c}}^{\mathfrak{a}} n_{\text{T}}^{\mathfrak{cb}} + w_{\mathfrak{c}}^{\mathfrak{b}} n_{\text{T}}^{\mathfrak{ac}} + \frac{dw_{\mathfrak{c}}^{\mathfrak{a}}}{d \ln k} \Gamma^{\mathfrak{cb}} + \frac{dw_{\mathfrak{c}}^{\mathfrak{b}}}{d \ln k} \Gamma^{\mathfrak{ac}} + \dots. \quad (2.24)$$

2.2 *Mathematica* implementation

In these grey panels we discuss the numerical *Mathematica* implementation of the transport method, available from transportmethod.com. In the control panel of this notebook one can specify the model to be evaluated and select which computations to perform.

Which observables?—By default, the notebook computes observables at a chosen scale k . Computing the spectral index at this scale using Eq. (2.18) on subhorizon scales requires delicate cancelations between oscillating terms. For some models it can be considerably slower than computing Σ^{ab} alone. In these cases it can be preferable to evaluate Σ^{ab} a few times (two is typically sufficient) and compute the spectral index *via* finite difference.^a

Power spectrum.—From the control panel one can also specify a range of k -scales at which to compute Σ^{ab} , in order to obtain the power spectrum as a function of scale $P_\zeta(k)$.

Example model.—Throughout this paper we use the 3-field model ‘number 2’ as an example. This is a simple extension of the case studied in Ref. [43], which is a model of quasi-single-field inflation giving rise to a feature in $P_\zeta(k)$ as a result of excitation of a heavy field via a nontrivial metric. (See §3 for a brief explanation of quasi-single-field scenarios.)

Number 2 can be regarded as a ‘quasi-two-field’ example. We add another light field to obtain, in addition to the nontrivial behaviour coming from $G^{\alpha\beta}$, superhorizon evolution *via* a turn in the plane of the two light directions. This turn arises in the region of field space where the metric is approximately the unit matrix. The turn occurs due to the hierarchy in the masses of the displaced fields — as the heavier field approaches its minimum, the direction of steepest descent becomes progressively more aligned with the lightest field. There is no direct motivation for this model, but at a qualitative level similar characteristics can arise in supergravity. Here we merely employ this example for illustrative purposes.

The model has an equation of motion of the form (2.3). The potential is

$$V = \frac{1}{2} \sum_{\alpha=1}^3 m_\alpha^2 \phi_\alpha^2 \quad (2.25)$$

and the mass ratios are $m_2^2/m_1^2 = 30$ and $m_3^2/m_1^2 = 1/81$. The metric takes the form

$$G^{\alpha\beta} = \begin{pmatrix} 1 & \Gamma & 0 \\ \Gamma & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad (2.26)$$

with

$$\Gamma \equiv \frac{0.9}{\cosh\left(2\frac{\phi_1^2 - 7}{0.12}\right)^2}. \quad (2.27)$$

^aFor practical purposes, however, it can be useful to solve Eq. (2.18) in order to understand how far inside the horizon we should start our computation; this will be discussed in §3.2. It is possible to select which method is used from the control panel.

3 Initial conditions

In a simple model we would typically apply (2.15) only in the superhorizon regime, where all masses are relevant because k/aH is exponentially small. We would estimate an initial value of Σ^{ab} for modes which are ‘light’ in the sense that k/aH dominates M_β^α/H^2 around horizon exit, and set all correlation functions to zero for ‘heavy’ modes to which this does not apply.

The justification is two-fold. First, heavy modes are orthogonal to the inflationary trajectory, so if this remains nearly straight throughout the epoch of horizon exit then fluctuations in these directions have no physical effect. Second, quantum fluctuations in massive modes decay exponentially, so they become irrelevant almost immediately.

Under certain circumstances this approximation may miss effects from modes with intermediate masses of order the Hubble scale or slightly larger. If bending of the inflationary trajectory is not negligible during horizon exit then fluctuations in massive modes can be partially converted into the adiabatic density perturbation before they have time to decay. Chen & Wang called this scenario ‘quasi-single field inflation’ [43–53]. It yields a distinctive bispectrum. Even if intermediate-mass modes are not relevant, turns in the field-space trajectory will cross-correlate fluctuations in different species. This can have a significant impact on the later evolution of observables. A striking example is the ‘destructive interference’ observed by McAllister, Renaux-Petel & Xu in Ref. [24].

As described in §2.1, we should account for all these effects by setting initial conditions sufficiently early that M^α_β/H^2 is negligible compared to $(k/aH)^2$. Because the transport equation requires no approximation to be made regarding M^α_β the subsequent evolution is exact (at tree level) and will capture all quasi-single field and cross-correlation effects.

In this section we explain how initial conditions can be computed in the deeply subhorizon regime, where all correlation functions are dominated by kinetic contributions.

3.1 Deep inside the horizon

In this section we work in conformal time, defined by $\tau = \int_\infty^t dt'/a(t')$.

Field correlation function.—In the massless limit, the Feynman two-point function evaluated in the vacuum state is⁹ [20]

$$\langle \delta\phi^\alpha(\mathbf{k}', \tau') \delta\phi^\beta(\mathbf{k}, \tau) \rangle = (2\pi)^3 \delta(\mathbf{k} + \mathbf{k}') \frac{\Pi^{\alpha\beta}(\tau', \tau)}{2k^3} H(\tau) H(\tau') (1 - ik\tau)(1 + ik\tau') e^{ik(\tau - \tau')}, \quad (3.1)$$

where we have assumed $\tau < \tau'$. The quantity $\Pi^{\alpha\beta}(\tau', \tau)$ is the parallel propagator evaluated on the inflationary trajectory,

$$\Pi^{\alpha\beta}(\tau', \tau) \equiv \text{P exp} \left(- \int_\tau^{\tau'} d\tau'' \Gamma^\alpha_{\lambda\mu}[\phi^\nu(\tau'')] \frac{d\phi^\lambda}{d\tau''} \right) G^{\mu\beta}(\tau). \quad (3.2)$$

It transforms as a bitensor; the index α transforms as a tensor in the tangent space at $\phi^\nu(\tau')$, whereas the index β transforms as a tensor in the tangent space at $\phi^\nu(\tau)$. The symbol P denotes path-ordering and rewrites its argument in order of decreasing time along the trajectory.

We take the equal-time limit $\tau = \tau'$ in which the parallel propagator reduces to the metric, and evaluate the correlation function well inside the horizon where $|k/aH| \approx |k\tau| \gg 1$. (If τ represents a time N e-folds prior to horizon exit for the mode k , then $|k\tau| \approx e^N$.) This yields

$$\langle \delta\phi^\alpha(\mathbf{k}) \delta\phi^\beta(\mathbf{k}') \rangle_\tau \approx (2\pi)^3 \delta(\mathbf{k} + \mathbf{k}') \frac{H^2 G^{\alpha\beta}}{2k^3} |k\tau|^2 \quad (3.3)$$

⁹The equal-time two-point function in a model with nontrivial field-space metric was calculated by Sasaki & Stewart [21]. The factor of the parallel propagator appearing in the unequal-time propagator was given in Ref. [20].

in which H and $G^{\alpha\beta}$ should be evaluated at the common time τ .

Vacuum state.—Eq. (3.3) gives a suitable initial condition for *all* field–field correlation functions at sufficiently early times, but only if we assume that the mode of wavenumber \mathbf{k} was practically in its vacuum state for at least a few e-folds before the time τ so that vacuum initial conditions were applicable.

This is not guaranteed. If inflation is sufficiently prolonged, a mode with fixed comoving wavenumber \mathbf{k} must have originated on very small physical scales. Physics at these scales is presumably not governed by the effective theory used to describe inflation, so these short-scale modes will join it only when they are redshifted within its purview. Their state at that time should properly be regarded as a boundary condition needed to define the effective field theory. Like all details of ultraviolet physics, it cannot be predicted from within the effective theory.

The influence of such boundary conditions was studied by Anderson, Molina-Paris & Mottola [54]. They found that, to be consistent with Einstein gravity as a low-energy description, the effective stress tensor generated by unobserved high-energy fluctuations should correspond to sufficiently depopulated occupation numbers at large frequencies. If these occupation numbers are conserved during redshifting then modes with these frequencies would join the effective description while practically in their vacuum state. In that case Eq. (3.3) will apply. This is the default assumption in many inflationary models.

An alternative, studied by a number of authors (see eg. Refs. [54, 55]), is that modes join the effective description at a fixed time before horizon exit with nonzero occupation number. In this case Eq. (3.3) would require corrections. Whether this occurs is a model-dependent question, but if corrections are necessary they can be accommodated as a change of initial conditions. The transport equations themselves do not require modification.

Correlation functions with momenta.—To compute correlation functions involving momenta we use the relation $dN = -d\tau/\tau$, which implies $\mathcal{D}_N = -\tau\mathcal{D}_\tau$. Differentiating the unequal-time field–field correlation function (3.1) and using that the parallel propagator is covariantly constant,

$$\mathcal{D}_{\tau'}\Pi^{\alpha\beta}(\tau', \tau) = \mathcal{D}_\tau\Pi^{\alpha\beta}(\tau', \tau) = 0, \quad (3.4)$$

we obtain the unequal-time field–momentum correlation functions,

$$\langle \delta\pi^\alpha(\mathbf{k}', \tau') \delta\phi^\beta(\mathbf{k}, \tau) \rangle = -(2\pi)^3 \delta(\mathbf{k} + \mathbf{k}') \frac{\Pi^{\alpha\beta}(\tau', \tau)}{2k^3} H(\tau) H(\tau') |k\tau'|^2 (1 - ik\tau) e^{ik(\tau - \tau')} \quad (3.5)$$

$$\langle \delta\phi^\alpha(\mathbf{k}', \tau') \delta\pi^\beta(\mathbf{k}, \tau) \rangle = -(2\pi)^3 \delta(\mathbf{k} + \mathbf{k}') \frac{\Pi^{\alpha\beta}(\tau', \tau)}{2k^3} H(\tau) H(\tau') |k\tau|^2 (1 + ik\tau) e^{ik(\tau - \tau')}. \quad (3.6)$$

We have neglected terms suppressed by the slow-roll parameter $\epsilon = -\dot{H}/H^2$, which are generated by differentiation of H . In (3.1) we did not retain slow-roll suppressed contributions (although this can be done), so retaining them here would give an inconsistent set of corrections. Also, we have again assumed $\tau < \tau'$. The case $\tau > \tau'$ can be obtained from these expressions by complex-conjugation.

The equal-time limit can be obtained as before, but unlike the field–field correlation function the result is complex. However, the imaginary part vanishes at late times and therefore does not affect observables. For simplicity we can work with the symmetrized (or ‘Weyl ordered’) correlation function which is always real and coincides with the other

field-momentum two-point functions outside the horizon,

$$\frac{1}{2}\langle\delta\pi^\alpha(\mathbf{k})\delta\phi^\beta(\mathbf{k}')+\delta\phi^\beta(\mathbf{k}')\delta\pi^\alpha(\mathbf{k})\rangle_\tau=-(2\pi)^3\delta(\mathbf{k}+\mathbf{k}')\frac{H^2G^{\alpha\beta}}{2k^3}|k\tau|^2. \quad (3.7)$$

By a very similar procedure, the momentum-momentum correlation function can be found (also to leading order in slow-roll terms) to be

$$\langle\delta\pi^\alpha(\mathbf{k})\delta\pi^\beta(\mathbf{k}')\rangle=(2\pi)^3\delta(\mathbf{k}+\mathbf{k}')\frac{H^2G^{\alpha\beta}}{2k^3}|k\tau|^4. \quad (3.8)$$

Collecting these results yields the *universal* initial conditions

$$\begin{aligned} \Sigma_*^{\alpha\beta} &= \frac{H_*^2 G_*^{\alpha\beta}}{2}|k\tau_*|^2, & \Sigma_*^{\bar{\alpha}\beta} &= \Sigma_*^{\alpha\bar{\beta}} = -\frac{H_*^2 G_*^{\alpha\beta}}{2}|k\tau_*|^2, & \Sigma_*^{\bar{\alpha}\bar{\beta}} &= \frac{H_*^2 G_*^{\alpha\beta}}{2}|k\tau_*|^4, \\ n_*^{\alpha\beta} &= H_*^2 G_*^{\alpha\beta} |k\tau_*|^2, & n_*^{\bar{\alpha}\beta} &= n_*^{\alpha\bar{\beta}} = -H_*^2 G_*^{\alpha\beta} |k\tau_*|^2, & n_*^{\bar{\alpha}\bar{\beta}} &= 2H_*^2 G_*^{\alpha\beta} |k\tau_*|^4 \end{aligned} \quad (3.9)$$

where a subscript ‘*’ denotes evaluation at the initial time.

As tensor modes behave like free scalar fields (apart from a change in normalization) their initial conditions follow immediately,

$$\begin{aligned} \Gamma_*^{\gamma\gamma} &= \frac{H_*^2}{M_{\text{P}}^2}|k\tau_*|^2, & \Gamma_*^{\pi\gamma} &= \Gamma_*^{\gamma\pi} = -\frac{H_*^2}{M_{\text{P}}^2}|k\tau_*|^2, & \Gamma_*^{\pi\pi} &= \frac{H_*^2}{M_{\text{P}}^2}|k\tau_*|^4 \\ n_{\text{T}*}^{\gamma\gamma} &= \frac{2H_*^2}{M_{\text{P}}^2}|k\tau_*|^2, & n_{\text{T}*}^{\pi\gamma} &= n_{\text{T}*}^{\gamma\pi} = -\frac{2H_*^2}{M_{\text{P}}^2}|k\tau_*|^2, & n_{\text{T}*}^{\pi\pi} &= \frac{4H_*^2}{M_{\text{P}}^2}|k\tau_*|^4. \end{aligned} \quad (3.10)$$

Slow-roll corrections.—In principle, the initial conditions (3.9) should be corrected by slow-roll terms proportional to powers of ϵ or its derivatives. Therefore although the transport equation (2.15) makes no use of the slow-roll approximation, our use of (3.9) *does* require that slow-roll is a fair approximation near the initial time. We do not need any form of the slow-roll approximation thereafter; the slow-roll conditions may be badly violated or fail entirely.

In certain cases it may happen that a solution with initial conditions chosen to satisfy Eq. (3.9) will still relax to the correct solution, even if slow-roll is only marginally valid or weakly violated near the initial time, provided we begin the calculation sufficiently far before horizon exit. As for any numerical solution, some care may be required to check that results are stable to changes in the grid and the initial time. In practical calculations this implies that the initial time should be chosen so that it is comfortably earlier than any interesting dynamical effects which we hope to capture.

3.2 *Mathematica* implementation

Increasing the number of e-folds of subhorizon evolution slows down the solver; but not starting the calculation sufficiently early leads to inaccurate results. The amount of subhorizon evolution (as well as the accuracy settings of the Mathematica function `NDSolve`) required to obtain a sufficiently accurate result is model dependent, however it is useful to have a prescription that works as a guideline.

One way to approach this is to use the behaviour of the spectral index. Sufficiently far inside the horizon, the dominant contribution to the scale dependence comes from $\Sigma_0^{\bar{\alpha}\bar{\beta}} \propto k^4$. Therefore we expect the spectral index $n_s - 1$ to be roughly 4 at early times, independent of the model. If the system is not given enough e-folds of subhorizon evolution, the delicate cancelations that occur for n_{ab} will quickly break and give $n_s - 1 \neq 4$. We have found that ensuring $n_s - 1 = 4$ for a sustained period of order ~ 3 e-folds is usually sufficient to obtain consistently good results. This method should not be used as a replacement for testing for convergence against changes in initial time and grid, but it can be used as an indicator.

4 Connection with observables

4.1 From field space to ζ

To calculate observables, the flat-gauge field and momentum correlation functions must be converted to correlation functions of the uniform-density gauge curvature perturbation ζ . Assuming all isocurvature modes decay, it is the curvature perturbation which sets initial conditions for density fluctuations in the later universe. In this section we briefly explain how an appropriate transformation can be extracted from the separate universe assumption using the methods of Ref. [56]. As explained there, the gauge transformation could equally well be derived from traditional perturbation theory in the large-scale limit.

Gauge transformation.—According to the construction of Ref. [56], the number of e-folds ΔN between a point p on a spatially flat hypersurface at which the density is ρ_p and an equivalent point on a nearby uniform density hypersurface with density ρ_* is

$$\Delta N = \left. \frac{dN}{d\rho} \right|_p (\rho_* - \rho_p) + \dots, \quad (4.1)$$

where the omitted terms are higher order in $\rho_* - \rho_p$. Under a variation of p , it follows that

$$\begin{aligned} \delta(\Delta N) &\approx - \left. \frac{dN}{d\rho} \right|_p \delta\rho_p + \dots \approx - \left. \frac{dN}{d\rho} \right|_p \left(\left. \frac{\partial\rho}{\partial\phi^\alpha} \right|_p \delta\phi_p^\alpha + \left. \frac{\partial\rho}{\partial\pi^\alpha} \right|_p \delta\pi_p^\alpha \right) + \dots \\ &\equiv N_\alpha \delta\phi^\alpha + N_{\bar{\alpha}} \delta\pi^\alpha + \dots, \end{aligned} \quad (4.2)$$

where ‘ \dots ’ denotes terms of higher order in $\delta\phi^\alpha$ or $\delta\pi^\alpha$ which are not needed for the first-order gauge transformation. The last equality should be interpreted as a definition of N_α and $N_{\bar{\alpha}}$. No use is being made of the slow-roll approximation so the density ρ contains both potential and kinetic contributions. Performing the partial derivatives, we find

$$N_\alpha = \frac{1}{2\epsilon} \frac{V_\alpha}{V} \quad (4.3a)$$

$$N_{\bar{\alpha}} = \frac{1}{2\epsilon(3-\epsilon)} \frac{\pi_\alpha}{M_P^2}. \quad (4.3b)$$

The variation $\delta(\Delta N)$ gives the fluctuation in e-folds required to reach ρ_* , and therefore must be the curvature perturbation ζ . It follows that Eq. (4.2) expresses the gauge transformation to ζ at linear order.

This argument was given in Ref. [20] to lowest order in the slow-roll approximation where the contribution for $\delta\pi^\alpha$ can be neglected. In the formulation given here, Eqs. (4.2) and (4.3a)–(4.3a) apply to all orders in the slow-roll expansion. The argument of Ref. [56], generalized to a nontrivial field-space metric, shows that if desired we can use the Hamiltonian constraint to eliminate the $\delta\pi^\alpha$ term. This would give

$$N_\alpha = -\frac{1}{2\epsilon} \frac{\pi_\alpha}{M_{\text{P}}^2} \quad (4.4a)$$

$$N_{\bar{\alpha}} = 0. \quad (4.4b)$$

Like (4.3a)–(4.3b), Eqs. (4.4a)–(4.4b) do not invoke the slow-roll approximation.

Power spectrum.—The quantity of principal interest is the power spectrum, which is defined in terms of the equal time $\zeta\zeta$ two-point function,

$$\langle \zeta(\mathbf{k}_1)\zeta(\mathbf{k}_2) \rangle = (2\pi)^3 \delta(\mathbf{k}_1 + \mathbf{k}_2) \frac{P_\zeta}{k^3}. \quad (4.5)$$

In terms of the flat-gauge correlation functions, it follows from Eq. (4.2) that P_ζ can be written

$$P_\zeta = N_a N_b \Sigma^{ab}. \quad (4.6)$$

The k -dependence of the power spectrum can be handled similarly. We define the scalar spectral index to satisfy

$$n_s - 1 \equiv \left. \frac{d \ln P_\zeta}{d \ln k} \right|_{k=k_*}, \quad (4.7)$$

where k_* is the pivot scale. (The subscript ‘ \star ’ representing evaluation at the pivot scale should not be confused with the subscript ‘ $*$ ’ denoting evaluation at the initial time in Eqs. (3.9).) We find

$$n_s - 1 = \frac{N_a N_b}{P_\zeta} \frac{d \Sigma^{ab}}{d \ln k} = \frac{N_a N_b n^{ab}}{N_c N_d \Sigma^{cd}}. \quad (4.8)$$

The running of the spectral index is defined to be

$$\alpha \equiv \left. \frac{d n_s}{d \ln k} \right|_{k=k_*}. \quad (4.9)$$

It can be computed using a finite-difference approximation, although another transport equation could be written for it if desired.

Tensor fraction.—The tensor power spectrum is defined by analogy with the scalar power spectrum

$$\langle \gamma_{ij}(\mathbf{k}_1) \gamma_{ij}(\mathbf{k}_2) \rangle \equiv (2\pi)^3 \delta(\mathbf{k}_1 + \mathbf{k}_2) \frac{P_\gamma}{k^3}. \quad (4.10)$$

The power in each polarization adds incoherently. Using the normalization condition $e_{ij}^s e_{ij}^{s'} = 2\delta^{ss'}$ it follows that the total tensor power satisfies

$$\langle \gamma_{ij}(\mathbf{k}_1) \gamma_{ij}(\mathbf{k}_2) \rangle = \sum_s \sum_{s'} \langle \gamma_s(\mathbf{k}_1) \gamma_s(\mathbf{k}_2) \rangle e_{ij}^s e_{ij}^{s'} = 2 \sum_s \langle \gamma_s(\mathbf{k}_1) \gamma_s(\mathbf{k}_2) \rangle. \quad (4.11)$$

Each polarization is the same and therefore the final result is $4\langle\gamma_+\gamma_+\rangle$, or equivalently $4\langle\gamma_\times\gamma_\times\rangle$. The tensor-to-scalar ratio r is defined to be

$$r \equiv \frac{P_\gamma}{P_\zeta} = \frac{4\Gamma^{\gamma\gamma}}{P_\zeta} \quad (4.12)$$

and the tensor spectral index is

$$n_T = \left. \frac{d \ln P_\gamma}{d \ln k} \right|_{k=k_*} = \frac{n_T^{\gamma\gamma}}{\Gamma^{\gamma\gamma}}. \quad (4.13)$$

4.2 End of inflation or beyond?

To complete the calculation, we must decide when to terminate the integration and measure final values for each observable.

In principle we should track the evolution of all correlation functions up to the last scattering surface—or until just before horizon re-entry if we wish to study the assembly of large-scale structure. In practice this is extremely challenging, partly because the results depend on the unknown details of reheating and partly because we have little direct knowledge of the epochs between reheating and horizon re-entry. (For recent literature studying the impact of reheating on inflationary observables, see Refs. [57–60]. Ref. [61] is a recent review of reheating in general.)

It is possible for ζ to evolve whenever power remains in any ‘isocurvature’ modes, by which we mean phase space directions transverse to the inflationary trajectory. Microwave background data now strongly constrain the presence of isocurvature modes around the time of photon decoupling at $z \sim 1100$, but this provides only a lower limit on the decay time. We would normally aim to terminate the integration as early as is safe, to avoid being obliged to integrate through periods of the universe’s history where we must make assumptions about its evolution. This means we must be able to determine when all power in isocurvature modes has become exhausted—what is called the ‘adiabatic limit’ [62, 63].

Isocurvature power during inflation.—First consider evolution during the inflationary era. One option would be to track the two-point functions of each relevant degree of freedom, using Gram–Schmidt orthogonalization to construct linear combinations which measure the power transverse to the inflationary trajectory. For practical purposes we could suppose that the system is close enough to an adiabatic limit whenever all of these two-point functions become sufficiently small.

This approach is feasible, but rather cumbersome. At least during slow-roll evolution an alternative is to use the optical analogy of trajectories flowing over field-space developed in Ref. [26]. When slow-roll is a good approximation there is no need to track momentum perturbations, and we can write an equation analogous to (2.14) purely for the field fluctuations,

$$\mathcal{D}_N \delta\phi^\alpha = w^\alpha{}_\beta \delta\phi^\beta, \quad (4.14)$$

where $w^\alpha{}_\beta$ is likewise an analogue of the expansion tensor (2.16),

$$w^\alpha{}_\beta = \mathcal{D}_\beta(\mathcal{D}_N \phi^\alpha) - \frac{1}{3} R^\alpha{}_{\gamma\lambda\beta} \mathcal{D}_N \phi^\gamma \mathcal{D}_N \phi^\lambda = \mathcal{D}_\beta \left(-\frac{V^\alpha}{3H^2} \right) - R^\alpha{}_{\gamma\lambda\beta} \frac{V^\gamma V^\lambda}{27H^4}. \quad (4.15)$$

Here, $V^\alpha = G^{\alpha\beta} V_\beta$. As explained in Ref. [26], the eigenvalues of $w^\alpha{}_\beta$ can be used to detect the presence of growing and decaying modes: a positive eigenvalue indicates a growing mode, whereas a negative eigenvalue indicates a decaying one.

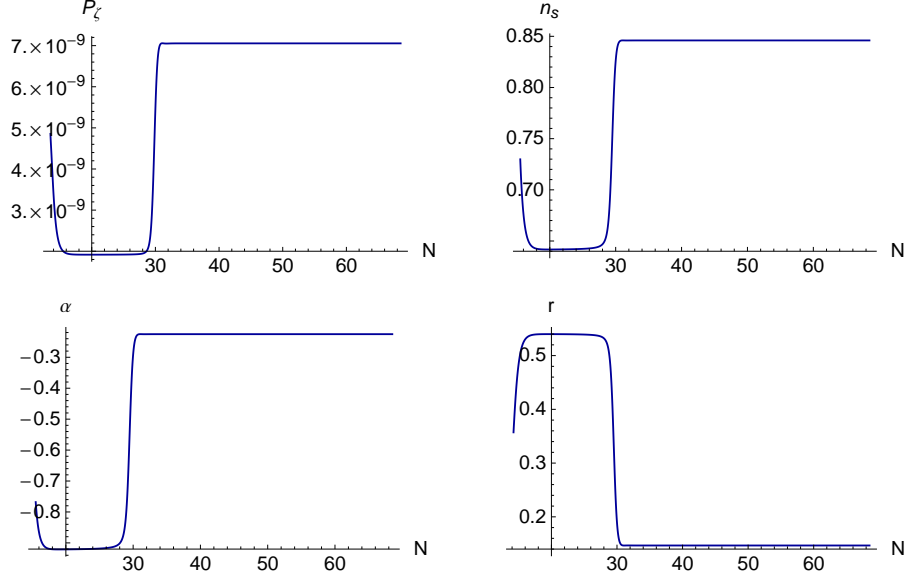


Figure 1. Evolution of observables as a function of e-folds N : clockwise from top left, the power spectrum P_ζ ; the spectral index n_s ; the running of spectral index α ; and the tensor-to-scalar ratio r .

In most circumstances one mode is constant or slowly evolving, and therefore gives an eigenvalue which is zero or slightly positive. Therefore, in an N -field system, approach to the adiabatic limit is signalled by the appearance of $N-1$ large negative eigenvalues. This method is simpler than computing all combinations of isocurvature correlation functions, but clearly shares its arbitrariness in deciding when the fluctuations have decayed sufficiently to declare that an adiabatic limit has been reached. There is always the possibility that extremely violent future dynamics could amplify even very small modes.

After inflation.—This test applies only during slow-roll evolution, and therefore will typically become unreliable some time *before* the end of inflation unless this is mediated by a sudden event such as a waterfall transition. When it applies, however, it may provide a rationale for terminating the integration at or before the end of the slow-roll phase. This is the best possible outcome.

Much less can be said if slow-roll breaks down before complete decay of the isocurvature modes. In this case, one should follow the decay of the scalar species relevant during inflation into reheating products. Isocurvature modes may be transferred or amplified during this process. One must then begin a second integration, following the evolution of these fluctuations using suitable phase space coordinates; normally, the scalar species supporting inflation will no longer be the relevant variables, and the transport equation for their correlation functions will need to be replaced. The range of phenomenology which can occur during this post-inflationary phase is comparatively under-explored, and almost certainly model-dependent.

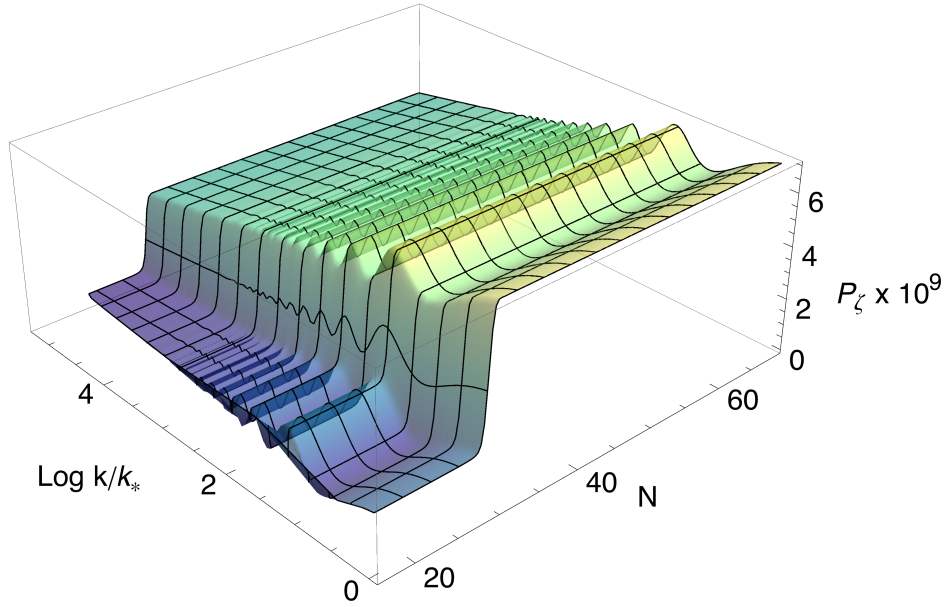


Figure 2. The power spectrum P_ζ as a function of e-folds N and wavenumber k . The range of scales corresponds to about 5 e-folds. Note the step in $P_\zeta(N)$ corresponding to superhorizon evolution, and the oscillatory features in $P_\zeta(k)$ as a result of excitations of the heavy mode around horizon exit.

4.3 *Mathematica* implementation

As above, we use the model Number 2 as an illustration.

Time dependence.—In Fig. 1 we plot the time evolution of the power spectrum, spectral index, running of the spectral index and tensor-to-scalar ratio for the scale leaving the horizon 55 e-folds before the end of inflation.

A turn in field space occurs after $N \sim 30$ e-folds. The turn causes isocurvature modes to source evolution of P_ζ , visible here as a large step. This corresponds to a sudden jump in the spectral index and running, and a corresponding drop in the value of the tensor-to-scalar ratio. Once the trajectory settles into the valley of the potential, no further evolution occurs.

Scale dependence.—In Fig. 2 we plot the time and wavenumber evolution of the function $P_\zeta(k)$. Evidently each scale undergoes qualitatively similar evolution to the example shown in Fig. 1. There is a significant step around $N \sim 30$. However, it is also possible to see the effect of excitation of the heavy mode: it induces oscillatory features in $P_\zeta(k)$ as a function of wavenumber.

Approach to the adiabatic limit.—We plot the time evolution of the eigenvalues of the slow-roll expansion tensor w^α_β in Fig. 3. Around horizon crossing the metric is designed to excite the heaviest field, leading to a sudden enhancement of the isocurvature modes, here visible as a sharp excursion to positive eigenvalues.

Soon after, one of the eigenvalues (the yellow line) becomes much more negative than the other two, indicating that isocurvature fluctuations associated with the heaviest field are decaying exponentially. The suppression is so rapid that the system is subsequently well-approximated by a two-field model.

After 20 e-folds of superhorizon evolution the trajectory turns, causing excitation of the remaining isocurvature mode. Its power is subsequently transferred to the adiabatic direction (approximately represented by the blue line), generating the step-like features in Fig. 1. After the turn the remaining isocurvature mode (the green line) is rapidly suppressed. At this point an adiabatic limit has been reached: the system has become effectively single-field, and ζ is conserved.

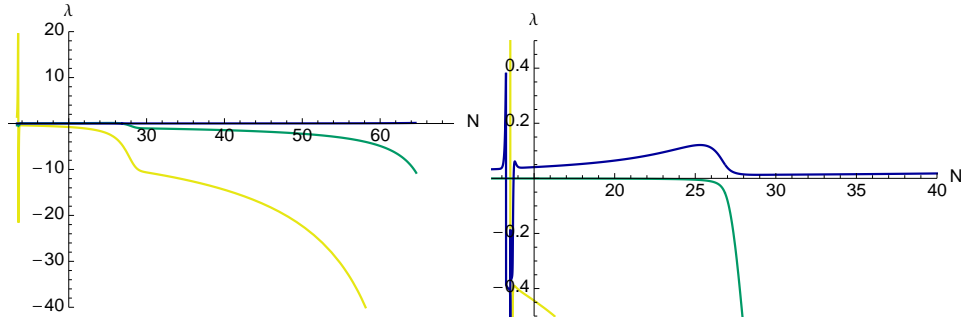


Figure 3. Eigenvalues of the slow-roll u^α_β as a function of number of e-folds. The left plot shows the whole evolution from horizon exit to the end of inflation. The right plot is zoomed in order to understand the transfer of power around the turn in field space.

5 Final summary

Computing precise predictions for observables in complex inflationary models requires tools going beyond textbook methods. This is especially true for models with a nontrivial field-space metric.

First, it is helpful (but not mandatory) to use a covariant description of the system, especially when computing correlation functions of higher-order (see, eg., Ref. [20]). Second, to track the influence of curvature scales associated with the metric we require a computational method which retains information about *all* mass scales in the problem. In this paper we describe a simple method for doing so, beginning with universal massless initial conditions long before horizon exit and solving a transport equation for the subsequent evolution. We have focused on the equal-time two-point functions because only these are required for the simplest inflationary observables. Nevertheless, only straightforward modifications are needed to compute unequal-time correlation functions or those of higher order.

This method is applicable to a large class of models, including models descending from ideas in string theory or supergravity where nontrivial field-space metrics are often associated with a nontrivial Kähler potential. It gives a simple description which allows the analysis to proceed from deeply subhorizon scales to the end of inflation (or beyond), with no matching required around the time of horizon exit. The evolutionary equation does not make use of the slow-roll approximation—although our analytic initial conditions do—and therefore accounts for effects from violation of the slow-roll conditions, turns in field-space at any point on the inflationary trajectory, and the influence of massive fields or quasi-single-field dynamics. It does not yet apply to models with entirely arbitrary kinetic terms, such as $P(X)$ or $P(X, \phi)$ models. We leave these for future work.

In this paper we have tried to explain how the transport method can be applied in practice to obtain predictions from inflationary models which exhibit one or more of these complexities. In addition we have attempted to highlight those points where our implementation goes beyond standard textbook methods such as the separate-universe approximation, and also those situations to which the method cannot yet be applied. In these cases we have indicated whether the obstruction is a matter of principle, or just an artefact of current technology. Since our focus is on practical usage, we have provided a complete *Mathematica* implementation which is used as an example. The code is intended to be accessible. We hope it will serve both as a useful tool for investigating realistic models, and a platform to extend the range of scenarios for which predictions can be obtained.

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